

1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-
2043-47-2 | DTXSID1062122

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.04

Global applicability domain: Outside

Local applicability domain index: 2.78e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

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1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 2.51

Predicted: 2.40

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o-Toluenesulfonamide

Measured: 2.57

Predicted: 2.00

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Benzotrifluoride

Measured: 44.7

Predicted: 13.7

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Benzenesulfonamide

Measured: 4.79

Predicted: 2.10

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Triallyl phosphate

Measured: 1.20

Predicted: 1.41